

# Machine Learning in the calibration process of Discrete Particle Model: The case with Angle of Repose

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## Abstract

This is where, stuff, happens. Literally. But not yet. Please wait.

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# 1 Introduction

Granular material is a family of material characterized by its large bulk of densely packed particles, ranging from nanometers to centimeters [1], and is able to resist deformation and form heaps, i.e., behave like a solid and withstand strong shear force [2]. Simple examples of granular materials include sand, gravel, clays, seeds, nuts, and all ranges of powders such as coffee powder, cement powder, which is shown in figure 1. Furthermore, many processes and equipments in chemical plants use granular materials, such as catalysis, adsorption, and heat exchangers. Granular materials are projected to make about half of the products and three-quarters of the raw materials used in the chemical industry [3]. Thus, understanding how granular materials behave is of great significance.



Figure 1: Examples of Granular Materials [4].

The simulation of granular material's bulk mechanical behavior is done using Discrete Particle Model (DPM, or Discrete Element Method - DEM), which generates the movement of individual particles to capture the macro-scale behavior. The DPM is a family of numerical methods for computing the motion of a large number of particles [5], first proposed by Cundall and Strack in the 1970s [6]. Since the properties of granular materials differ wildly, these simulations require an extensive calibration process designed individually for each type of granular material. Some parameters of the granular material model can be measured directly, such as size distribution or density. However, other parameters are effective parameters (i.e., they result from a simplified particle model) and thus cannot be directly measured. These parameters are then calibrated by choosing a few standard calibration setups (rotating drum, heap test, ring shear cell) and simulating these setups in a DPM simulation, and the missing parameters are determined such that the response of the experimental and simulation setups match.

Recently, coupled with the raise of Machine Learning in other fields, it has also been applied to solve the calibration problem. This has been done using a Neural Network [7, 8, 9, 10], Genetic Algorithm [11], and a recursive Bayesian sequential Monte-Carlo filtering algorithm named GrainLearning [12]. In this Assignment, three Machine Learning algorithms will be discussed: Neural Network, Random Forest (supervised model), and GrainLearning (unsupervised model). These three algorithms set to treat the calibration problem in two different ways, and likewise, solve it in two different ways: While GrainLearning looks to identify the microparameters from the experimental and DEM simulations's bulk parameters (inverse problem), the supervised models will help generating a database that can map different microparameters combinations to their corresponding bulk parameters, generated by DEM simulations. In other word, NN and RF will learn the built-in relationship between the micro- and macroparameters of the Discrete Particle Model, thus allow a much faster prediction compare to a full DEM simulation. One advantage of GrainLearning compares to other Machine Learning algorithms such as Neural Network is that it is an unsupervised learning algorithm, i.e., it can starts calibrating

with a minimal amount of input information. However, each material needs calibration for multiple bulk parameters, i.e., Static Angle of Repose, Dynamic Angle of Repose, shear tester, etc. since a set of microparameters that is valid for one bulk parameter might not valid for another. Therefore, scaling up with a Neural Network model might be more simple, since a Neural Network can produce multiple valid combinations for each bulk parameter.

In the next section, the characterisation and experimental method will be discussed, including static Angle of Repose, Discrete Particle Model, contact laws, and the material used in the simulation. Section 4 will discuss in detail different approach and method of each model. The result of GrainLearning will be discussed in section 5, while section 6 discuss the supervised model's performance. Subsequently, section 7 will compare the models, discuss the strength and weakness of each model, and the limitations.

## 2 Characterisation of granular materials

There is no established standard of characterisation measurements for granular materials. Typical measurements include heap test, rotating drum test, linear/ring shear cell test, and the silo flow test..., in which the output is the bulk parameter, which defines how the granular material behaves in large quantity - such as the angle of repose (AoR), shear stress, flow rate.

This research is focused on one of the essential bulk parameters to describe the characteristics of the granular materials - the static angle of repose. Static AoR, described in Fig. 2, is defined as the angle that granular solids form when it is piled with a flat surface and is essential to characterise the coarseness and smoothness of materials. This, in turn, can help design a process involved with the material - lower static AoR implies more flowable and thus easier to transport with less energy [13].

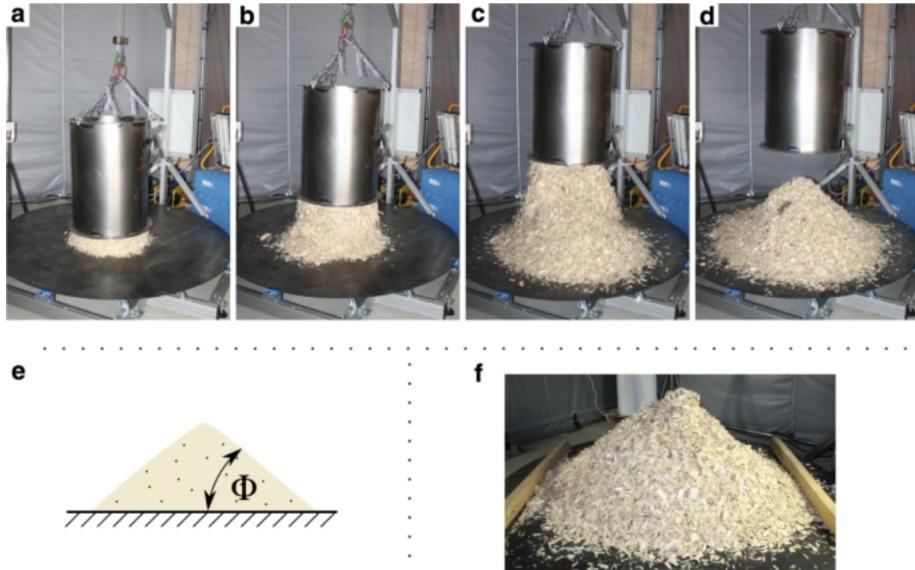


Figure 2: Static Angle of Repose measurement steps [14].

## 3 Simulation Method

### 3.1 Discrete Particle Model

Discrete Particle Model simulates particle motion by applying forces and torques which derives from particle-particle interactions and external influences, on the basis of the given contact law. It performs calculations of kinematics that a given particle  $i$  exerts on other particle  $j$ , for each particle in the

system, among with the peripheral factors such as gravity and walls. To achieve this results, the particles are assumes to be (1) undeformable - deform therefore implemented as overlap, (2) unbreakable, (3) all internal interactions are due to particle-particle interaction, (4) Each particle pair  $i, j$  has only one contact point  $c_{ij}$  which the forces and torques act on, and (5) all external forces and torques are either body forces and torques or by interacting with a wall [15].

### 3.1.1 Contact Laws

For each particle  $i$  on the system, Eq. 1 describes the internal and external forces, and Eq. 2 describes the torque acting on it [15]:

$$F_i = \sum_{j=1}^{n_p} F_{ij} + \sum_{k=1}^{n_w} F_{ik}^w + F_i^b \quad (1)$$

$$\tau_i = \sum_{j=1}^{n_p} r_{ij} F_{ij} + \tau_{ij} + \sum_{k=1}^{n_w} r_{ik} F_{ik}^w + \tau_{ik}^w + \tau_i^b \quad (2)$$

With  $F_{ij}$  interparticle forces,  $F_{ik}^w$  the interaction force between each wall and the particle,  $n_p$  = number of particles,  $n_w$  = number of walls,  $F_i^b$  body forces i.e., gravity, and  $r_{ij}$  as the branch vector, which connects the particle position  $r_i$  with the contact point  $c_{ij}$ . The same hold for torques equation, with  $\tau$  as torque.

The contact law used in the simulations is the Linear Spring-Dashpot model, implemented in MercuryDPM as `LinearViscoelasticFrictionReversibleAdhesiveSpecies`. It defines the interaction between two particles  $i$  and  $j$  as a damped harmonic oscillator [16]:

$$F_{ij}^n = \begin{cases} k_n \delta_{ij}^n + \gamma_n v_{ij}^n & \text{if } \delta_{ij}^n > 0, \\ 0 & \text{else,} \end{cases} \quad (3)$$

In this equation,  $k_n > 0$  represents spring stiffness,  $\gamma_n \geq 0$  represents the damping coefficient,  $v_n$  the normal vector, and  $\delta_{ij}^n$  is the overlap between the particles. Two particles interact with each other if and only if they overlap. This contact model is simple, has an analytic solution, and is less computationally expensive [17], while also suitable for large particles [15]. In addition to particle-particle interactions, the current contact law also takes into account sliding friction, rolling friction, and adhesion. While sliding friction is defined as the force that acts in the tangential direction between two particles when they collide and resist lateral motion, rolling friction resists the angular motion of the particles (see equation 4, 5).

$$|F_{ij}^t| \leq \mu^l F_{ij}^n \quad (4) \quad \tau_{ij}^{\text{ro}} \leq \mu^{\text{ro}} \alpha_{ij}^{\text{eff}} F_{ij}^n \quad (5)$$

With  $F_{ij}^t$  and  $\tau_{ij}^{\text{ro}}$  as the forces in the tangential direction, and rolling torques, respectively. When the lateral forces reach a particular threshold, the particle will begin to slide. The sliding motion is modelled using the Coulomb yield criterion, which cuts off the elastic displacement when it reaches a specific fraction (sliding friction  $\mu^l$ ) of the normal force. The same applies to the rolling torque: it is cut off when it reaches a certain level, defined by the rolling friction  $\mu^{\text{ro}}$ . Finally, the adhesive forces model is defined as:

$$F_{ij}^a = \begin{cases} -F_{\max}^a & \text{if } \delta_{ij}^n > 0, \\ -F_{\max}^a - k_c \delta_{ij}^n & \text{if } -F_{\max}^a/k_c \leq \delta_{ij}^n < 0, \\ 0 & \text{else,} \end{cases} \quad (6)$$

The adhesive forces are reversible, i.e., equal during loading and unloading. The maximum adhesion force  $-F_{\max}^a$  is calculated using the bond number:

$$F_{\max}^a = gm_{50}\text{Bo} \quad (7)$$

With  $g$  denotes the gravitational acceleration, and  $m_{50}$  is the average mass of the particles. More details about the sliding, rolling friction, and adhesion can be found in [15] and [16].

### 3.1.2 Angle of Repose measurement

In MercuryDPM, Static AoR is measured by a hollow cylinder simulation, which consists of two cylinders (instead of one cylinder and one plate in Fig. 2), with the cylinder's diameter. For simplicity, all particles in the simulation are assumed to be a perfect sphere. After all the particles are poured into the cylinder, it is let to rest until the bulk's kinetic energy is less than 1% compared to the potential energy (steady-state condition). At this point, the top cylinder is removed, and all the particles that have fallen out of the bottom cylinder below  $z = 0$  are deleted. This will result in a cone-shaped heap of particles and a drastic increase in kinetic energy due to gravity. The heap will be rested again until it reaches a steady-state condition as mentioned above, and then Static AoR can be measured. The measurement will be done twice, since the kinetic energy of the system can be increased again after the first measurement. Figure 3 demonstrates an example simulation of MercuryDPM.

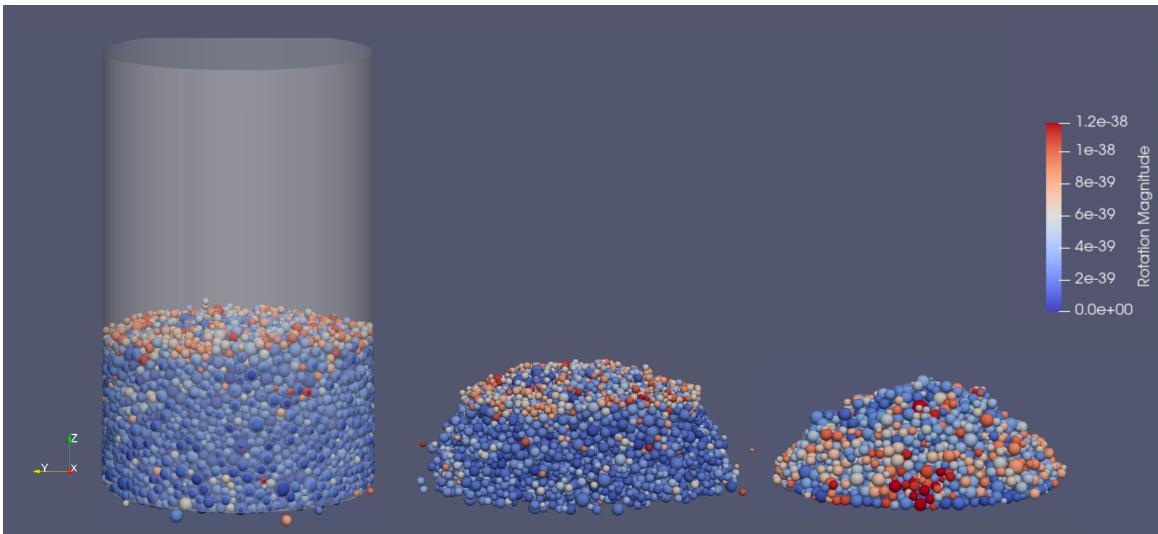


Figure 3: Angle of Repose simulation on MercuryDPM. From left to right: Initial fill stage, wall removed, and final stage.

## 3.2 Material and simulation properties

Experimental data on quartz sand is provided by Derakhshani et al. [18]. The density of quartz sand is  $\rho = 2653 \text{ kg/m}^3$ , and the particle size distribution (PSD) given in Table 1, with the static AoR of  $33^\circ$ . Meanwhile, experimental data on limestone is provided by Shi et al. [19], specifically the Eskal 150 limestone, since this material has a similar static AoR and density ( $33^\circ$  and  $2761 \text{ kg/m}^3$ ), while the PSD is in a much lower range.

Material	Diameter ( $\mu\text{m}$ )	Cumulative volume distribution (%)
Limestone	97	10
	138	50
	194	90
Quartz sand	300	6.21
	425	24.50
	500	50.55
	600	100

Table 1: Particle Size Distribution of materials.

The experimental data described above will be used as constant input values for each DEM simulation. In addition, four variables - including three described in eq. 4, 5, and 7 will be tested to determine their respective static AoR: Restitution coefficient, sliding friction, rolling friction, and bond number. The restitution coefficient is the ratio between the particle's velocity before and after the collision. The parameter range of restitution coefficient is 0 to 1, with 1 denoting a perfectly elastic collision. All other microparameters has a positive bound - the value ranging from 0 to  $\infty$ ; however, in most realistic case, the value is also smaller than 1.

## 4 Calibration of Discrete Particle Model

### 4.1 GrainLearning

GrainLearning is a calibration toolbox developed by Cheng et al., utilizes the recursive Bayesian algorithm to estimate the uncertainty parameters in DPM. Initially, a wide range of parameter space is quasi-randomly sampled from the initial guess range to create a prior distribution of each parameter. Then, conditioned on the experimental values, the posterior distribution of the parameters is updated recursively by Sequential Monte-Carlo Filtering (SMC Filter) and fitted to a Gaussian Mixture Model. This process is done iteratively, until a desired value that minimises the loss function is reach, typically 3 iterations. Algorithm 1 and the following sections will describe in brief the calibration workflow implemented in GrainLearning.

#### 4.1.1 Posterior distribution calculation

Initially, the measurement is assumed to have an error represented by a covariance matrix  $\Sigma_\alpha = \sigma \omega_\alpha y_\alpha$ , with  $\sigma$  the covariance parameter, and important weight of the measurement  $\omega$ . With  $\Sigma$ , the likelihood of a given state  $\Theta_k^{(i)}$ , i.e., the probabilistic prediction to the experimental data  $y$  can be estimated by the multivariate normal distribution, with  $y_t$  measurement data at time step t, and  $d$  the dimension of the state vector  $\Theta_k^{(i)}$ :

$$p(y_t | \Theta_k^{(i)}) \propto \frac{1}{(2\pi)^{d/2} |\Sigma|} \exp \left( -\frac{1}{2} (y_{kt} - x_{kt}^{(i)})^\top \Sigma^{-1} (y_{kt} - x_{kt}^{(i)}) \right) \quad (8)$$

With the calibration system being modelled as a hidden Markov model, the posterior distribution of  $\Theta_k^{(i)}$  can be calculated using recursive Bayes' rule:

$$p(\Theta_k^{(i)} | y) \propto \prod_{t=1}^{N_t} p(y_t | \Theta_k^{(i)}) p(\Theta_k^{(i)}) \quad (9)$$

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**Algorithm 1** GrainLearning

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**Input:**

- $\mathbf{y}$ : Experimental values
- $\mathbf{x} = \mathbf{F}(\Theta)$ : DEM solver
- $(\Theta_{min}, \Theta_{max})$ : Initial guess range

**Main:**

- ▷ Set uniform prior distribution:  $p(\Theta) = \mathcal{U}(\Theta_{min}, \Theta_{max})$
- for**  $k$  in range  $(0, K)$  **do**

  - ▷ Sampling parameters:
  - if**  $k = 0$  **then** sample  $N_p$  parameters values from initial distribution:  $\Theta_k^{(i)} \sim p_0(\Theta)$
  - else if**  $k > 0$  **then** sample  $N_p$  parameters values from prior distribution:  $\Theta_k^{(i)} \sim p_{k-1}(\Theta | y_{1:T})$
  - ▷ Evaluate DPM:  $x_k^{(i)} = F(\Theta_k^{(i)})$
  - ▷ Optimizing  $\sigma$ :
  - while** True **do**

    - ▷ Compute likelihood (Eq. 8):  $p(y_t | \Theta_k^{(i)}) \propto \mathcal{N}(y_{kt} | x_{kt}^{(i)}, \Sigma)$
    - ▷ Compute posterior distribution of  $\Theta_k^{(i)}$  conditioned to  $y$  (Eq. 9).
    - ▷ Compute Effective Sample Size (ESS) with Eq. 10.
    - ▷ Stop if target ESS value is reached:
    - if**  $k = 0$  and  $ESS > 20\%$  **then** break
    - else if**  $k > 0$  and  $ESS \sim ESS_{max}$  **then** break
    - ▷ Fit sampled posterior distribution to Gaussian Mixture Model:  $p(\Theta | y) = \sum_{\alpha}^k \lambda_{\alpha} \mathcal{N}(\mu_{\alpha}, \sigma_{\alpha})$
    - ▷ Set new prior distribution:  $p(\Theta) \leftarrow p(\Theta | y)$

**Output:**  $\Theta_{opt}$  in  $\Theta_K$  that minimizes  $|F(\Theta_{opt} - y)|$

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#### 4.1.2 Effective multi-level sampling

The Effective Sample Size (ESS) is calculated by summing the posterior distribution squared of all the sampled parameters value  $N_p$ :

$$ESS = \frac{1}{N_p \sum_{i=1}^{N_p} p(\Theta_k^{(i)} | y)^2} \quad (10)$$

The main idea is to draw the sample from the previously acquired knowledge about the relationship between  $\Theta$  and  $y$ . In the first iteration ( $k = 0$ ), The uniform prior distribution is chosen as the proposal density, and the parameter spaces are drawn from there. Subsequently, for  $k > 0$ , the proposal density will be the posterior distribution from the previous iteration  $p(\Theta | y)$ . After each iterations, the sampling space will get narrower - therefore, to ensure a proper proposal density for the sampling of parameters, the optimization process will be continued until appropriate  $\sigma$  which maximizes ESS is reached.

#### 4.1.3 Identification of microparameters with GrainLearning

In the first iteration of calibration, GrainLearning will initialize a set of parameter combinations using Halton sequence, from the initial guess range provided. This set of parameters will be passed to MercuryDPM to analyze with a Heap test, after which a static AoR is produced. From this data, GrainLearning will compute the next set of parameters on the basis of the previous MercuryDPM output, according to algorithm 1. For each attempt, GL will be running for 4 iterations - except when the simulations of that iteration takes more than two days, and that attempt will be classified as failed.

## 4.2 Neural Network

Artificial Neural Network (ANN) is a set of algorithms that seeks to identify correlations in data utilizing a technique inspired by how the human brain operates - mimicking how each neuron in the brain signals each other. The most basic ANN model is the Feed-forward Multilayer Perceptron Neural Network (MLPNN), in which the purpose is to define the mapping between the input and output

$y = f(x; \theta)$  and approximate the parameter  $\theta$  which results in the best possible function. In MLPNN, the data will flows in one direction from the input to the output, hence the name feed-forward. Like other supervised learning algorithms, an MLPNN needs to be trained before accurately describing the input and output relations. This is typically done by feeding the network with pre-labeled data, comparing the model's output with the desired output, and updating the weights parameter  $\theta$  - a process called backpropagation. In this assignment's context, Neural Network (NN) will be used when referring to Feedforward Multilayer Perceptron Neural Network, and NN models implemented in this research are provided by the open-source library `TensorFlow` [20].

#### 4.2.1 Designing a Neural Network

There are no general rules for determining the number of layers and the number of neurons per layer, and it depends heavily on each use case. While Benvenuti et al. [7], He et al. [8], and Daniel et al. [9] used only a single-layer ANN and varied the number of neurons, Ye et al. [10] vary both. However, the ultimate goal in both case is to find the combinations which result in the minimum error while also avoiding overfitting, i.e., the model excels on training but perform poorly on the validation step. In this case, for each simulation material, 250 models ranging from 2 to 15 layers and 5 to 15 neurons per layer are tested to determine the best model. Each model is trained for 50 epochs with a batch size of 32, and the metric used to grade the model is Mean Absolute Error. The optimization algorithm used is Adam [21], which are easy to configure, combine the best features of other optimization algorithm, and works robustly in most cases. In addition, 20% of the data will be saved for validation of the model.

Another important component of a Neural Network is the activation function. Since each neuron performs calculation by multiplying the input with weight and adding a bias, the activation function's role would be introducing a non-linearity element into an otherwise linear neuron. According to Goodfellow et al. [22], Rectified Linear Unit (ReLU) is the recommendation for most Deep Learning models, with its ability to preserve much of the properties due to its near-linear shape. ReLU activation function is defined as  $f(x) = \max(0, x)$ .

### 4.3 Random Forest algorithm

This section will discuss different concepts of a Random Forest (RF) algorithm, starting with the basis of the RF: decision tree. Decision tree is an algorithm that generates a tree graph of decisions based on the input provided and their possible outcomes, and as a consequence, it partitions the input space into multiple regions, with each region accounting for a different outcome [23]. An example of a simple decision tree based on two inputs is shown in figure 4.

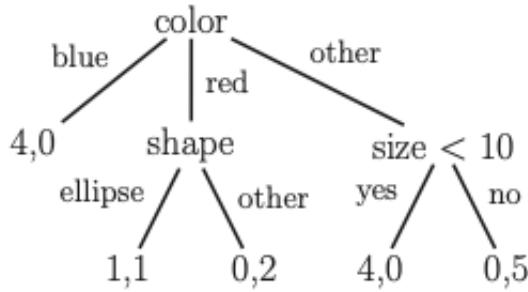
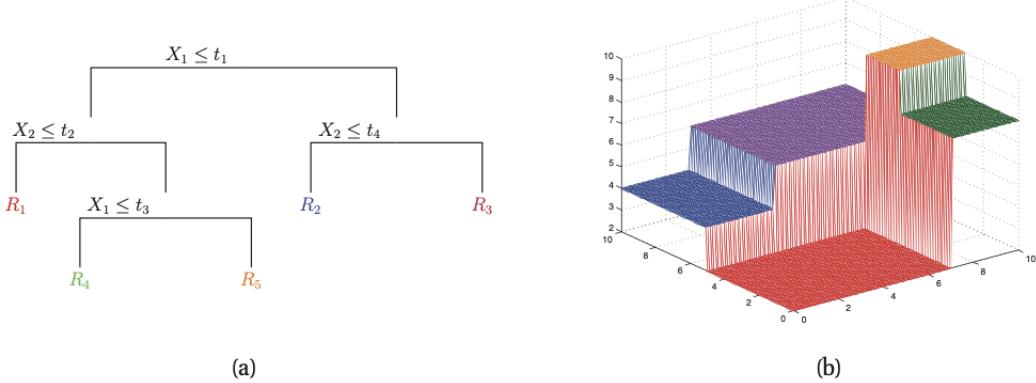


Figure 4: Example of a decision tree regressor on a two-input problem. [23]

The most significant advantage of the decision tree, and subsequently, random forest algorithm, is that it is relatively simple, explainable, easy to train and interpolate with little computational resources. However, one crucial drawback of a decision tree is its instability: minor data changes might affect the tree structure, making the decision tree a high variance estimators [23]. Attempts have been made to reduce the uncertainty of the decision tree, one of which is the so-called Random Forest algorithm, which Breiman proposed in 2001 [24]. RF made up for the high variance of a single decision tree by averaging the results over a “forest” of decision trees, with each tree represents an independent sampled vectors. The concept of decision tree and RF, therefore, fit within the scope of the calibration problem.

#### 4.4 Training and evaluation method for supervised models

To train the NN and RF model, 500 DEM simulations with randomized combinations of input parameters have been performed, in order to create a database which maps DEM microparameters to static AoR. Other 125 simulations did not finish on the time constraint set, and as a results marked as an inaccurate combination.

## 5 GrainLearning evaluation

Material	Quartz Sand			Limestone		
Attempt	1	2	3	1	2	3
Restitution Coefficient	[0.5 1]	[0 1]	[0 1]	[0.5 1]	[0.5 1]	[0 1]
Rolling Friction	[0 1]	[0 0.5]	[0.5 1]	[0 1]	[0 0.5]	[0.5 1]
Sliding Friction	[0 1]	[0 0.5]	[0.5 1]	[0 1]	[0 0.5]	[0.5 1]
Bond number	[0 1]	[0 0.5]	[0.5 1]	[0 1]	[0 0.5]	[0.5 1]

Table 2: Calibration attempts using GL

To analyse the performance of GL in calibrating DPM, multiple attempts has been made for each materials. In each attempt, the search range of the microparameters changed

Table 2 gives details on different calibration attempts with GL for two materials mentioned above: quartz sand and limestone. The difference between each attempt is that the search range of the microparameters changed. The first attempt serves as the control for both materials, while the second and the third are set up in smaller ranges. Overall, approximately 200 DEM simulations were performed for quartz sand, and 3 produced a valid combination. For limestone, 300 DEM simulations were performed, and five are valid. The valid combinations are marked in bold on the result tables in the following section.

### 5.1 Limestone

The calibration results by GL for limestone are described in table 3, and the details on how the sampling algorithm performs, i.e., conditioned on the previous simulation, is the sampled parameters for the next iteration make the simulation result converge to the experimental result, are described in figure 5. In the third calibration attempt, the second iteration did not finish in time due to the system's high level of kinetic energy; therefore, only iteration 1 is shown. In the control attempt, initially, only four iterations were performed. However, one remarkable observation is that GL clusters over the combinations produce a static AoR around  $40^\circ$ . This is reflected in the second iteration's result, where the best combination results in a static AoR of  $39.4803^\circ$ . Moreover, although the third iteration's result is  $33.0979^\circ$ , this seems like an outlier of the cluster. Therefore, an additional iteration was performed - and the results here verify the observation. The closest value to experimental static AoR is  $31.5243^\circ$ , and it is also the outlier of the cluster.

After the first calibration attempt, it is clear that the combinations that would result in the desired static AoR lie around  $0.8 - 1.0$  for restitution coefficient and in the lower-0.25 range for the rest of the contact parameters. Therefore, two more attempts were performed, with different initial ranges: attempt 2 with sliding friction, rolling friction, and bond number ranging from 0 to 0.5. With attempt 3, the sliding friction, rolling friction, and bond number range from 0.5 to 1, while the restitution coefficient's range is widened to 0 to 1.

As expected, the second attempt's performance was the most robust, reaching a near-perfect solution at the end of iteration 4. The clustering of the optimal result can also be seen clearly in figure 5. Meanwhile, the results from the third attempt verify the conclusion from the first attempt about the range of the optimal parameters - with higher rolling friction, sliding friction, and bond number, the static AoR reaches a maximum value of around  $65^\circ$ .

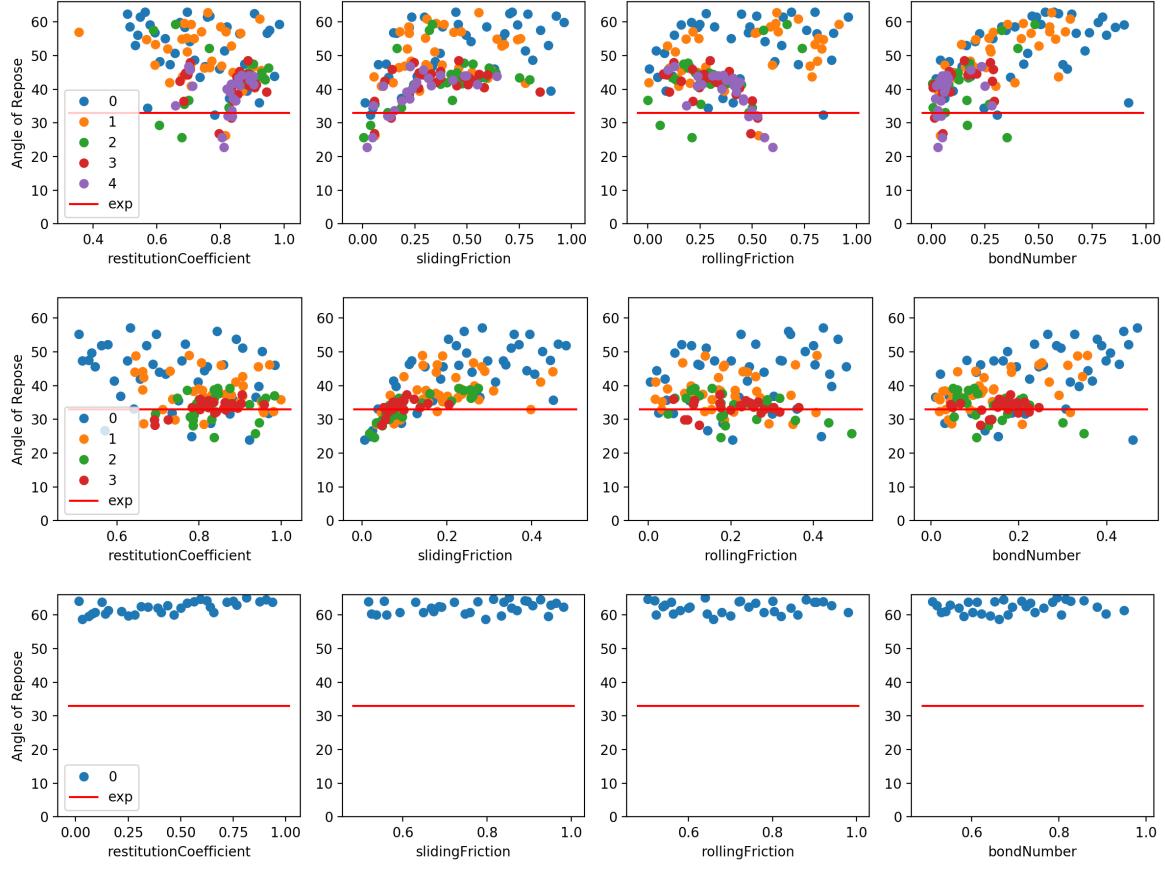


Figure 5: *From top to bottom*, attempt 1, 2, and 3 at calibrating Eskal with GL. Scatter dots with different colors denote each iteration, and red line denotes experimental value.

Attempt/Iter	Restitution Coefficient	Sliding Friction	Rolling Friction	Bond number	Result AoR
1.1	0.7812	0.037	0.84	0.3061	32.3163
1.2	0.869	0.2725	0.3652	0.0325	39.4803
1.3	0.831	0.1194	0.484	0.064	33.0406
1.4	0.8332	0.135	0.5262	0.0137	31.5243
1.5	0.8348	0.1517	0.497	0.0297	33.6745
2.1	0.6406	0.037	0.36	0.3061	33.0979
2.2	0.9546	0.3983	0.032	0.0334	32.9993
2.3	0.8263	0.0917	0.2226	0.1411	34.1421
2.4	0.8025	0.0710	0.2802	0.1748	32.9812
3.1	0.0312	0.7963	0.66	0.6632	58.6606

Table 3: Calibration results of limestone with GL.

## 5.2 Quartz sand

The calibration result for quartz sand is given in table 4, and the parameters sampling graph is given in figure 6. In the control attempt, only the first iteration is shown, partly due to 6/40 simulations of the second iteration does not finish in time, but also due to the results of the second iteration does not cluster at the experimental value, with most averaging around  $45^\circ$  to  $50^\circ$ . Due to the similarity between

quartz sand and limestone in terms of experimental static AoR, the second attempt of quartz sand will be initialized with the same range as the second attempt of limestone. And as a result, attempt 2 has the best performance out of the three. One noticeable thing here is that the rolling friction has two different clusters identified by GL instead of one, compared to sliding friction, restitution coefficient, or bond number. This denotes the multi-solution phenomena of a calibration problem since there could be more than one combination that can produce a sufficient static AoR - which is shown in iterations 3 and 4 of attempt 2: the rolling friction for iteration 3 is 0.07, while for iteration 4 is 0.41. Different experiments, i.e., Shear Cell test or Drum test (Dynamic AoR), would be needed in addition to the heap test to find an ideal combination of microparameters. However, this is out of the scope of the current research.

In the third attempt, although the range was specified as shown in table 2, the Gaussian Mixture Model algorithm of GL sampled some of the values in iteration 3 and 4 outside the initial range. This was a known bug in the current GL version implemented in MercuryDPM. Therefore, it was able to generate a correct combination with very low sliding friction, which results in a static AoR of  $34.2227^\circ$ , remarkably close to the experimental value.

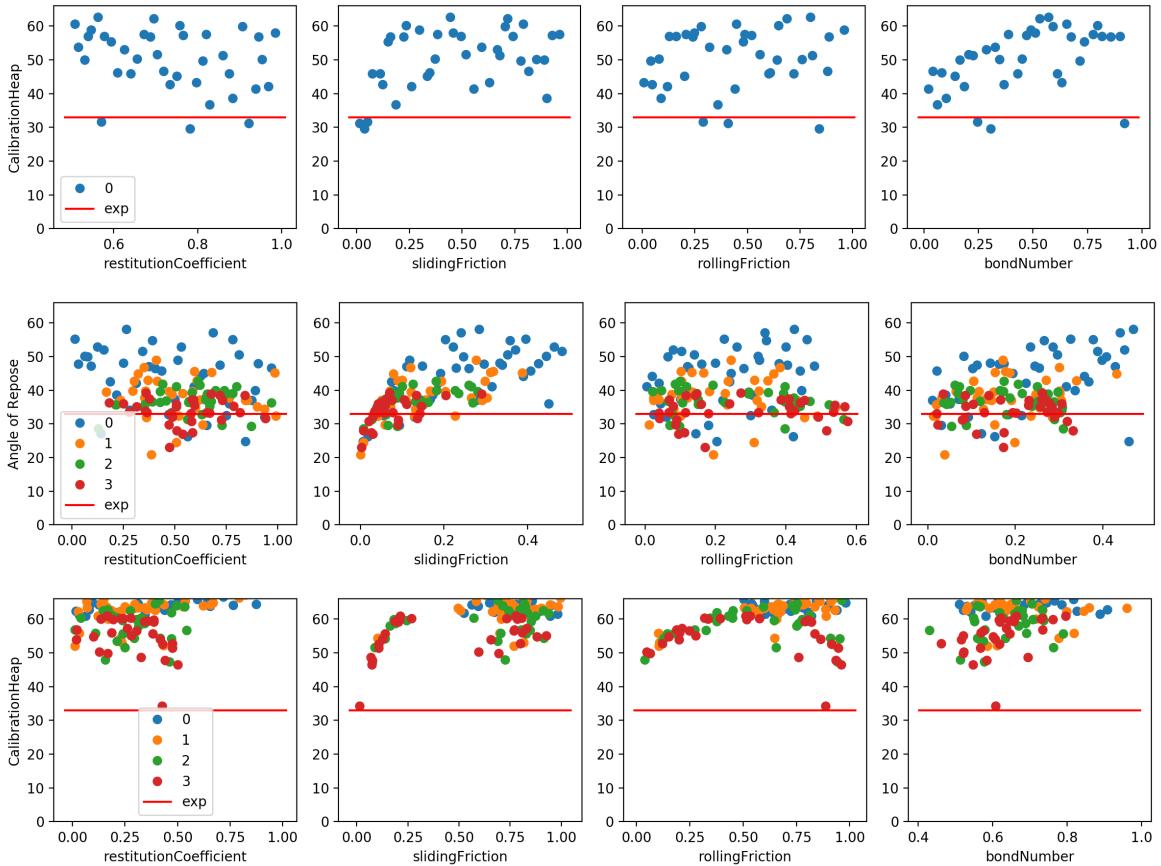


Figure 6: *From top to bottom*, attempt 1, 2, and 3 at calibrating quartz sand with GL. Scatter dots with different colors denote each iteration, and red line denotes experimental value.

### 5.3 Discussion

Overall, GL has demonstrated the capability to identify the ‘cluster’ in all calibration cases that the initial ranges were correctly defined - the combinations after each iterations are sampled closer and closer to the experimental value, as shown in attempt 2 of limestone and quartz sand. However, it has also shown inconsistent performance: In attempt 1 of limestone, the algorithm seeks to cluster in the range of  $35^\circ$  to  $45^\circ$ .

Attempt/Iter.	Restitution Coefficient	Sliding Friction	Rolling Friction	Bond number	Result AoR
1.1	0.5703	0.0493	0.288	0.2448	31.6303
2.1	0.4688	0.0617	0.024	0.1836	32.8394
2.2	0.992	0.2261	0.0987	0.0126	32.3687
2.3	0.6307	0.0606	0.0787	0.1795	32.8670
2.4	0.4800	0.0321	0.413	0.2946	33.0521
3.1	0.0625	0.9444	0.82	0.5816	60.9714
3.2	0.0109	0.7683	0.1052	0.5853	52.0551
3.3	0.4604	0.0752	0.9406	0.5777	47.3408
3.4	0.427	0.0146	0.8872	0.6075	34.2227

Table 4: Calibration results of sand with GL.

## 6 Supervised model evaluation

In this section, the performance of the two supervised models, i.e., Neural Network and Random Forest, is investigated for limestone and quartz sand, respectively. For the NN model, over 800,000 different combinations, as described in table 5, has been processed - and over 2,000,000 for RF model. Any combinations that produce a static AoR within the 0.1% margin of error to the experimental data are marked as a correct combination. This combination will then be evaluated independently by a DEM simulation to verify the ability of supervised models to correctly describe a material's bulk behaviour based on the given contact law.

	Restitution Coefficient	Sliding Friction	Rolling Friction	Bond number
Range	[0.5 1]	[1e-5 1]	[1e-5 1]	[1e-5 1]
Number of values (NN)	30	30	30	30
Number of values (RF)	38	38	38	38

Table 5: Random evenly-spaced microparameters combinations

### 6.1 Limestone

For limestone, 12 over 800,000 combinations of DEM input parameters processed by the ANN was a ‘valid’ combination: the output of the ANN was  $33 \pm 0.01^\circ$ . Meanwhile, with 2,000,000 million combinations processed by RF, 22 of them were valid combinations - however, many of them are closely similar with a minor difference in one of the micro parameters, and only nine are distinct. The valid combinations are described in table 6 and 7, with figure 7 illustrates the combinations and their respective output. Overall, the NN model has correctly identified three combinations, while the Random Forest model has 2.

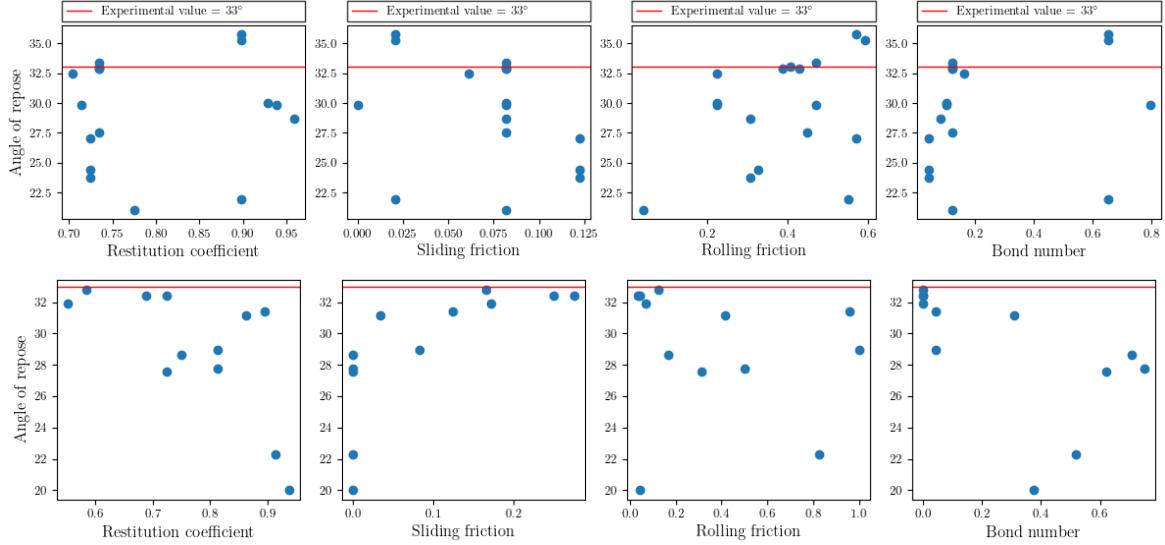


Figure 7: *From top to bottom*, valid contact law parameters identified by Random Forest and Neural Network model for limestone, and their respective simulation results.

Restitution coefficient	Sliding friction	Rolling friction	Bond number	Angle of repose
<b>0.6875</b>	<b>0.2500</b>	<b>0.0417</b>	<b>0</b>	<b>32.4263</b>
0.7500	0	0.1667	0.7083	28.6156
<b>0.5833</b>	<b>0.1667</b>	<b>0.1250</b>	<b>0</b>	<b>32.7926</b>
0.5517	0.1724	0.0690	0	31.9425
0.8125	0.0833	1.0000	0.0417	28.9393
<b>0.7241</b>	<b>0.2759</b>	<b>0.0345</b>	<b>0</b>	<b>32.3962</b>
0.8958	0.1250	0.9583	0.0417	31.4044
0.8621	0.0345	0.4138	0.3104	31.1331
0.7241	0	0.3104	0.6207	27.5978
0.8125	0	0.5000	0.7500	27.7676
0.9138	0	0.8276	0.5172	22.2677
0.9375	0	0.0417	0.3750	20.0361

Table 6: Valid contact law parameters identified by the NN model for limestone and their respective simulation results.

Restitution coefficient	Sliding friction	Rolling friction	Bond number	Angle of repose
<b>0.7041</b>	<b>0.0612</b>	<b>0.2245</b>	<b>0.1633</b>	<b>32.4872</b>
0.7245	0.1225	0.5714	0.0408	27.0585
<b>0.7347</b>	<b>0.0816</b>	<b>0.4082</b>	<b>0.1225</b>	<b>33.0331</b>
0.7347	0.0816	0.4694	0.1225	33.3593
0.7755	0.0816	0.0408	0.1225	21.0172
0.8980	0.0204	0.5714	0.6531	35.7342
0.9286	0.0816	0.2245	0.1020	29.9625
0.9592	0.0816	0.3061	0.0816	28.6865
0.7143	0	0.4694	0.7959	29.8154

Table 7: Valid contact law parameters identified by the RF model for limestone and their respective simulation results.

## 6.2 Quartz Sand

It is noteworthy that the quartz sand model was trained with less simulations compare to limestone model, with 322 DEM simulations. However, the performance of NN model when predicting the correct combinations that results in a static AoR of  $33^\circ$ : 4 out of 10 combinations are valid after verified by a full DEM simulation. Meanwhile, while the RF model predicts 20 different combinations, only 3 of them were valid - but interestingly, most of the combinations predict by RF model ranging very close to the experimental value, from  $29^\circ$  to  $31^\circ$ . The number of combinations passed to NN and RF model for quartz sand is approximately the same as for limestone.

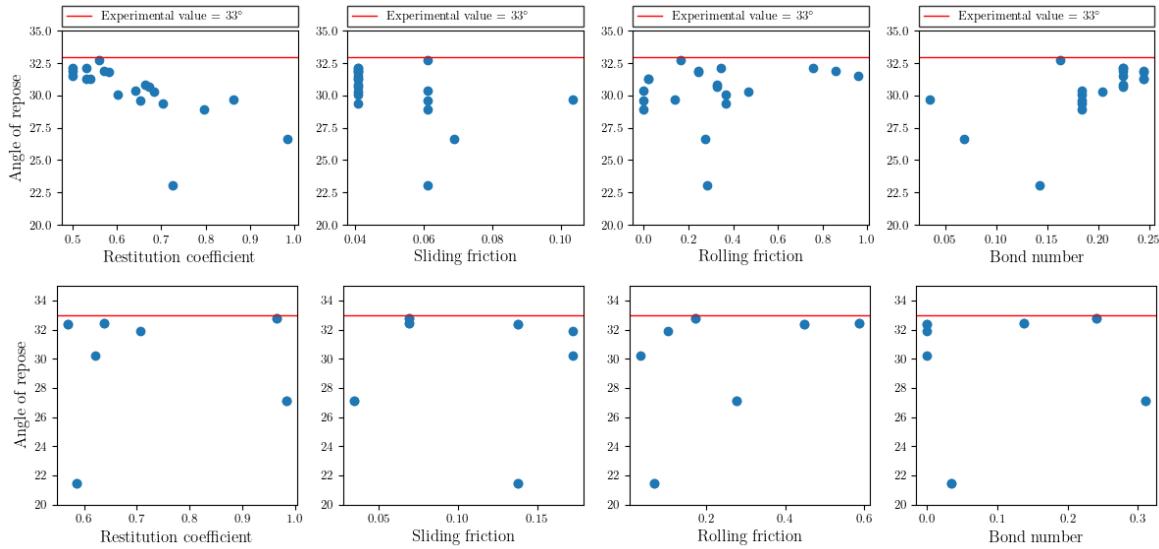


Figure 8: *From top to bottom*, valid contact law parameters identified by Random Forest and Neural Network model for quartz sand, and their respective simulation results.

Restitution coefficient	Sliding friction	Rolling friction	Bond number	Angle of repose
<b>0.5690</b>	<b>0.1379</b>	<b>0.4483</b>	<b>0</b>	<b>32.3822</b>
0.7069	0.1724	0.1035	0	31.9092
0.6207	0.1724	0.0345	0	30.2535
<b>0.6379</b>	<b>0.0690</b>	<b>0.5862</b>	<b>0.1379</b>	<b>32.4170</b>
0.5862	0.1379	0.0690	0.0345	21.4586
<b>0.9655</b>	<b>0.0690</b>	<b>0.1724</b>	<b>0.2414</b>	<b>32.7969</b>
0.9828	0.0345	0.2759	0.3104	27.0953
0.5862	0.1379	0.0690	0.0345	21.4586
<b>0.9655</b>	<b>0.0690</b>	<b>0.1724</b>	<b>0.2414</b>	<b>32.7969</b>
0.9828	0.0345	0.2759	0.3104	27.0953

Table 8: Valid contact law parameters identified by the NN model for quartz sand and their respective simulation results.

Restitution coefficient	Sliding friction	Rolling friction	Bond number	Angle of repose
<b>0.5612</b>	<b>0.0612</b>	<b>0.1633</b>	<b>0.1633</b>	<b>32.7325</b>
<b>0.5000</b>	<b>0.0408</b>	<b>0.7551</b>	<b>0.2245</b>	<b>32.1187</b>
0.5000	0.0408	0.8571	0.2245	31.8814
<b>0.5306</b>	<b>0.0408</b>	<b>0.3469</b>	<b>0.2245</b>	<b>32.1125</b>
0.6429	0.0612	0	0.1837	30.3771
0.5714	0.0408	0.2449	0.2449	31.8564
0.6020	0.0408	0.3674	0.1837	30.0461
0.5408	0.0408	0.0204	0.2449	31.2764
0.5000	0.0408	0.9592	0.2245	31.5459
0.5816	0.0408	0.2449	0.2449	31.8087
0.6531	0.0612	0	0.1837	29.6271
0.7041	0.0408	0.3674	0.1837	29.3786
0.6633	0.0408	0.3265	0.2245	30.8579
0.5306	0.0408	0.0204	0.2449	31.2787
0.6735	0.0408	0.3265	0.2245	30.6531
0.7959	0.0612	0	0.1837	28.9042
0.6837	0.0408	0.4694	0.2041	30.2650
0.7245	0.0612	0.2857	0.1429	23.0546
0.8621	0.1035	0.1379	0.0345	29.6629
0.9828	0.0690	0.2759	0.0690	26.6594

Table 9: Valid contact law parameters identified by the RF model for quartz sand and their respective simulation results

### 6.3 Discussion

In the current approach, NN and RF models have demonstrated the ability to capture the bulk DPM behavior and generate a database that can then be used to interpolate bulk parameters. Due to limited training data, it is not expected that the models would have a high accuracy in the interpolation step, so a validation step is needed. However, the current number of valid combinations does not meet the expectations of a calibration problem. This can be seen in the quartz sand’s RF model: multiple combinations that have been marked as valid by the model have either the same sliding friction or bond number - and this is the case for the NN model with limestone as well. One possible solution for this is to extend the ‘valid’ combination range from the current  $33 \pm 0.001$  - however this will result in a lot more valid combinations and thus only be possible if combined with other bulk tests to reduce the number of verification simulations. Only the combinations that produce satisfactory value in all bulk tests will be verified with DEM simulations.

Another limitation of the supervised approach is that each trained model only account for a single contact law - in this case is the linear-spring dashpot model. If the current contact law is not appropriate to describe the granular material, choosing another contact law would require a completely new model.

## 7 Model comparision

One of the most important factor in the calibration process of DPM is computational efficiency, since each DEM simulation is very costly in term of resources (for a static AoR, the simulation time varies from 2 to 24 hours each, and other simulations such as Dynamic AoR, shear cell test are even more expensive).

The current calibration routine using GL for static AoR costs around 120 to 150 DEM simulations, depends on how many iterations are needed. And most of the time, GL will delivers an adequate solution - except the first attempt with limestone as mentioned in section 5, where GL sampled combinations clusters in the wrong location. Meanwhile, with the current implementation of supervised models, 300 to 500 DEM simulations would be neccessary to train the models, and about 20 more are neccessary to verify the combinations that supervised models output (training and interpolating time are not taken into account here since they are negligible compare to simulation time).

However, computational efficiency would not be the only factor in weighing different method, since this approach of calibration (matching DEM bulk value with experimental bulk value) has no unique solution, i.e., a combinations of microparameters that works

one of the main point: computational efficiency. -Assume a calibration with GL cost 40 DEM simulations per iteration, for each bulk parameter it would be 7-8 iterations 300 DEM simulations =  $\zeta$  less DEM simulations, fully automatic, has been proven for more complex contact laws.

- For limestone, the amount of DEM simulations used to train NN and RF are 485, and for quartz sand are 322. The numbers are slightly higher than GL, but the performance are more robust from a small experiment: Produces multiple valid combinations per bulk parameter, therefore easier to identify the correct one by comparision with other bulk parameter's combinations.

- Limitations of RF: has not been tested against complex contact laws

Throughout multiple calibration routines with GrainLearning, it is identified that the initial guessing range played a key role in the ability of GL to idenitfy the correct set of micro-parameters.

## 8 Conclusion

## 9 Further recommendations

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